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Exact solution of an exclusion model in the presence of a moving impurity on a ring

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Abstract. We study a recently introduced model by Arndt *et al* which consists of positive and negative particles on a ring. The positive (negative) particles hop clockwise (anticlockwise) with unit rate and oppositely charged particles may swap their positions with asymmetric rates q and unity. In this paper we assume that a finite density of positively charged particles ρ and only one negative particle (which plays the role of an impurity) exist on the ring. It turns out that the canonical partition function of this model can be calculated exactly using matrix product ansatz formalism. In the limit of infinite system size and infinite number of positive particles, we can also derive exact expressions for the speed of the positive and negative particles, which show a second-order phase transition at $q_c = 2\rho$. The density profile of the positive particles on the ring has a shock structure for $q \leqslant q_c$ and an exponential behaviour with correlation length ξ for $q \geqslant q_c$. It will be shown that the mean-field results become exact at $q = 3$ and no phase transition occurs for $q > 2$.

1. Introduction

One-dimensional driven diffusive systems have provided a rich framework for the study of many interesting phenomena such as phase transitions, shock structures and the spontaneous breaking of translational invariance in the context of non-equilibrium statistical mechanics [1–4]. Moreover, from the mathematical point of view, some of them are related to the integrable quantum chain Hamiltonians and can be mapped to other non-equilibrium models, for instance, interface growth and traffic flows [5, 6].

In this paper, we study a recently introduced exclusion model which exhibits both phase transition and spatial condensation of particles [8, 9]. In this model two types of particle, called *positive* and *negative*, occupy the sites of a periodic one-dimensional lattice of length L. The particles are subjected to hard-core exclusion, so that there are three possible states at each site: empty or occupied by a positive particle or by a negative one. The positive (negative) particles hop to their immediate right (left) site with unit rate provided that it is empty. Adjacent positive and negative particles also exchange their positions with asymmetric rates q and unity. Therefore, during the infinitesimal time step dt, any bond $(i, i+1)$ (with $1 \leqslant i \leqslant L$) evolves

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as follows:

$$
\begin{array}{lll}
(+)(0) \rightarrow (0)(+) & \text{with} & \text{rate } 1 \\
(0)(-) \rightarrow (-)(0) & \text{with} & \text{rate } 1 \\
(+)(-) \rightarrow (-)(+) & \text{with} & \text{rate } q \\
(-)(+) \rightarrow (+)(-) & \text{with} & \text{rate } 1.
\end{array}
\tag{1}
$$

With periodic boundary conditions, the stationary state of this model has been studied by Monte Carlo simulation, the mean-field approximation and recently using analytical approaches in the neutral case in which the densities of the positive and negative particles are equal [8–11]. It has been shown that in the neutral case the model possesses two different phases depending on the reaction rate q [10], in contrast to the analytical results of [11], which indicate that there is no such transition. This model has also been studied with open boundaries in two special limits [12].

Here we study this model in the charged case in which a finite density of positive particles ρ and only one negative particle are present on the ring. Using the matrix product ansatz (MPA) formalism first introduced in [7], we can derive the exact analytic expression for the partition function of this model. Exact calculations show that in the limit of infinite system size and infinite number of positive particles the model has two different phases for $q < 2$, and the transition point q_c depends on the density of the positive particles. Exact expressions for the speed of the positive and negative particles can also be computed in this limit. We will see that these expressions have different behaviours depending on the value of q. For $q \leqslant q_c$, the speed of the positive and negative particles, as a function of q, increases linearly with q from zero. However, for $q \geqslant q_c$ the speed of the positive particles remains constant while the speed of the negative particle still increases as a function of both ρ and q. The speed of particles as a function of q is continuous at the transition point although its derivative changes discontinuously at this point. Also for $q \geqslant q_c$ it turns out that the density profile of the positive particles has an exponential behaviour with a characteristic length $\xi = |\ln \frac{q_c}{q}|^{-1}$, while the system presents a shock, i.e. a sharp discontinuity between a region of high density of particles and a region of low density for $q \leqslant q_c$. At the transition point the correlation length diverges and the model shows a second-order phase transition. We will show that at $q = 3$ the stationary probability of all possible configurations become equal. At this point no correlation exists and mean-field results are exact [8].

This paper is organized as follows. In the section 2, we obtain the exact expression for the canonical partition function of the model using the MPA. In section 3, we derive exact expressions for the speed of both kinds of particle, and also for the density profile of the positive particles on the ring. In the last section we compare our results with those obtained from the neutral case.

2. Expression of the canonical partition function using the MPA

According to the MPA formalism [7], the stationary probability distribution $P(\{C\})$ of any configuration $\{C\}$ can be expressed as a trace of a product of non-commuting operators. For the model proposed here we assume that there are M positive particles and only one negative particle on a ring of length L. Since this model is translationally invariant, we can always keep the single negative particle at site L and write the normalized stationary probability distribution as

$$
P(\{C\}) = \frac{1}{Z_{L,M}} \operatorname{Tr}\left(\prod_{i=1}^{L-1} (\tau_i D + (1-\tau_i) E) A \right) \tag{2}
$$

where $\tau_i = 1$ if the site i is occupied by a positive particle and $\tau_i = 0$ if it is empty. The matrices D, A and E which stand for the presence of a positive and a negative particle and a hole satisfy the following algebra introduced in [10]:

$$qDA - AD = D + A \tag{3}$$

$$DE = E \tag{4}$$

$$EA = E. \tag{5}$$

The normalization factor $Z_{L,M}$, which plays the role analogous to the partition function in equilibrium statistical mechanics, ensures that $\sum_{\text{all conf.}} P(\{C\}) = 1$ and can be written as a trace

$$Z_{L,M} = \mathrm{Tr}(G_{L,M}A) = \mathrm{Tr}\left(\sum_{\{\tau_i=0,1\}} \delta\left(M - \sum_{i=1}^{L-1} \tau_i\right) \prod_{i=1}^{L-1} (\tau_i D + (1-\tau_i)E)A\right). \tag{6}$$

Here $\delta(x)$ is the Kronecker $\delta_{x,0}$. In fact, the expression (2) is a conditional probability distribution which gives the probability of finding configuration $\{C\}$ in the stationary state provided that a negative particle exists at site L. We will see that all the physical quantities such as the speed of particles and the density profile of the positive particles can be written in terms of $Z_{L,M}$. It can easily be checked that a one-dimensional representation of the algebra (3)–(5) exists

$$D = A = E = 1$$

for $q = 3$ [8]. In this case (as can be seen from (2)) all configurations of the system occur with equal probabilities $P(\{C\}) = \frac{1}{Z_{L,M}}$ and no correlation exists. It implies that at $q = 3$ the mean-field results are exact. We will see that in this case $Z_{L,M}$ is equal to the total number of all possible configurations of the system. Traditionally, one has to find the representations of the algebra appears in MPA formalism and use it to calculate both the partition function and physical quantities, but in this paper we show that (see the appendix) the expression (6) can be calculated directly using the algebra (3)–(5) and has a closed form

$$Z_{L,M} = \sum_{i=0}^{M} \frac{(q-3)(\frac{2}{q})^i + 1}{q-2} C_{L-i-2}^{M-i} \tag{7}$$

in which $C_i^j = \frac{i!}{j!(i-j)!}$ is the binomial coefficient. At $q = 3$ we have

$$Z_{L,M} = \sum_{i=0}^{M} C_{L-i-2}^{M-i} = C_{L-1}^{M}$$

which is simply the total number of possible configurations of the model.

3. Exact physical quantities

In the stationary state, the speed of the positive particles in the reference frame of the lattice is found to be (see the appendix)

$$V_+ = \frac{(L-M)Z_{L-1,M-1} + C_{L-2}^{M-1}}{MZ_{L,M}}. \tag{8}$$

Similarly, the speed of the negative particle in the reference frame of the lattice can be obtained (see the appendix)

$$V_- = \frac{Z_{L-1,M-1} + C_{L-2}^{M} + C_{L-2}^{M-1}}{Z_{L,M}}. \tag{9}$$

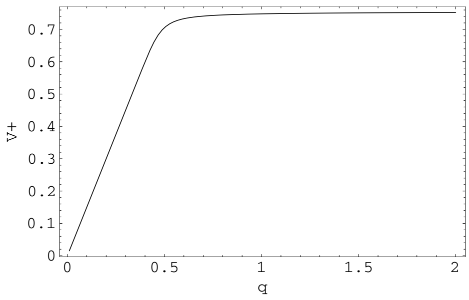

Figure 1. The speed of the positive particles V_+ as a function of q for $\rho = 0.25$ (plot of equation (8)). The phase transition takes place at $q_c = 0.5$.

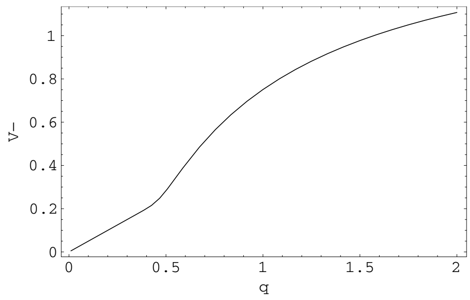

Figure 2. The speed of the negative particle V_- as a function of q for $\rho = 0.25$ (plot of equation (9)). The phase transition takes place at $q_c = 0.5$.

In figures 1 and 2 we have plotted V_+ and V_-, respectively, computed from the exact expressions (8) and (9) as a function of q for $L = 500$ and $M = 125$. As can be seen the behaviour of these functions changes near $q_c = 2\rho$. However, we should take the limit ($L, M \to \infty$ and $\frac{M}{L-1} = \rho$ being fixed) to find the exact transition point. We use the steepest descent method for computing the transition point. At this limit the asymptotic behaviours of (8) and (9) are given by

$$V_+ = \begin{cases} \frac{q}{2}\left(\frac{1-\rho}{\rho}\right) & \text{if} \quad 2\rho \geqslant q \\ 1-\rho & \text{if} \quad 2\rho \leqslant q \end{cases} \tag{10}$$

$$V_- = \begin{cases} \frac{q}{2} & \text{if} \quad 2\rho \geqslant q \\ \rho + \frac{1}{1+\frac{\rho}{q-2}-\frac{\rho(q-2)}{q-2\rho}} & \text{if} \quad 2\rho \leqslant q. \end{cases} \tag{11}$$

Thus, the transition point is exactly found to be $q_c = 2\rho$. Now it is obvious that for $q > 2$ no phase transition can take place because of the restriction on the density $\rho < 1$.

To study the nature of these phases we can compute the density profile of the positive particles on the ring. The average density of the positive particles $n(x)$ at the distance x from the negative particle is equal to the probability of finding a positive particle at site $L - x - 1$. Using the same procedure as proposed in the appendix, it can be shown that

$$n(x) = \frac{Z_{L-1,M-1} - \frac{q-3}{2}\{\sum_{i=1}^{M-x}(\frac{2}{q})^{x+i} C_{L-(x+i)-2}^{M-(x+i)}\}\Theta(M \geqslant x)}{Z_{L,M}} \tag{12}$$

where

$$\Theta(y \geqslant x) = \begin{cases} 1 & \text{if} \quad y \geqslant x \\ 0 & \text{otherwise.} \end{cases} \tag{13}$$

As can be seen from (12) the density profile of positively charged particles is completely flat at $q = 3$. In what follows we study the density profile (12) in the thermodynamic limit.

3.1. *Power-law phase;* $2\rho \leqslant q$

In this phase, as can be seen from figure 3, the negative particle has a short-range effect on the system. The density profile starts from $n(0)$ just in front of the negative particle and

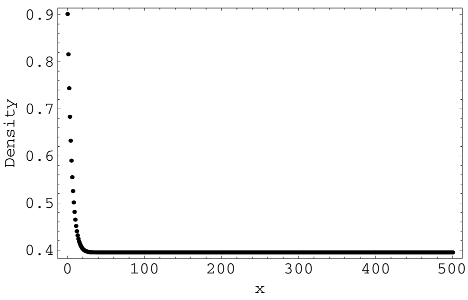

Figure 3. The density profile of the positive particles $n(x)$ for $L = 500$, $M = 200$ and $q = 0.95$ (plot of equation (12)). The negative particle is at $x = 0$.

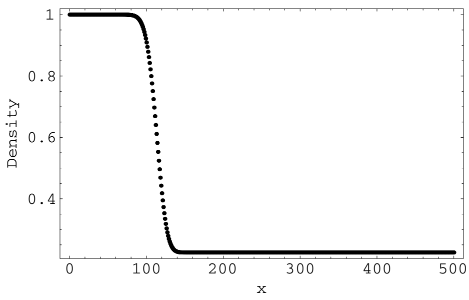

Figure 4. The density profile of the positive particles $n(x)$ for $L = 500$, $M = 200$ and $q = 0.45$ (plot of equation (12)). The negative particle is at $x = 0$.

decreases exponentially to its bulk value ρ. The asymptotic behaviour of formula (12) in the limit ($L, M \to \infty$ and $\frac{M}{L-1} = \rho$ being fixed) is given by

$$n(x) = \rho \left(1 - \frac{(1-\rho)(q-2)(q-3)}{(q-2)(q-2\rho) - \rho(q-2\rho) - \rho(q-2)^2} \mathrm{e}^{-\frac{x}{\xi}} \right) \tag{14}$$

in which $\xi = |\ln \frac{q_c}{q}|^{-1}$ specifies the disturbance due to the existence of the negative particle.

3.2. Jammed phase; $2\rho \geqslant q$

In this domain, the negative particle provokes a macroscopic shock in the system, as can be seen in the figure 4. A high-density region $\rho_{\mathrm{High}} = 1$ extending from $x = 0$ to $x = x_0$ is separated by a sharp interface from a region of low density $\rho_{\mathrm{Low}} = \frac{q}{2}$ extending from $x = x_0$ to $x = L - 1$. The position of the shock x_0 can be obtained from the thermodynamic behaviour of (12) in this region

$$x_0 = L \frac{q - 2\rho}{q - 2}.$$

4. Comparison and concluding remarks

In this paper we investigated a recently introduced model [8, 9] in the special limit of infinite system size and infinite number of positively charged particles in the presence of one negative particle. In this limit, the model shows both a phase transition and spatial condensation of particles in one dimension. The phase transition takes place at $q_c = 2\rho$, between a power law and a jammed phase. The speeds of the positive and the negative particles are not differentiable at the transition point $q_c = 2\rho$. In the neutral case, when the densities of the positive and negative particles are equal, the model shows a first-order phase transition at $q_c = \frac{1+6\rho}{1+2\rho}$, where the density of particles as a function of fugacity has a finite jump [8, 10]. Very recently it has been shown that the transition point can be determined, with great accuracy, using Yang–Lee theory in the non-equilibrium context [10]. In [10] the author presents a numerical study, using the grand canonical ensemble, but in contrast to the original Yang–Lee paper does not give a proof of the existence or nonexistence of the phase transition. Although it was claimed that such a transition does not exist in the framework of either a grand canonical or canonical ensemble [11], our exact calculations admit that in the limit ($L, M \to \infty$ and $\frac{M}{L-1} = \rho$ being fixed) the phase transition exists and in comparison to the neutral case [8] the transition point is shifted. In the neutral case the current of both positive and negative particles is zero for $q < 1$ where the particle segregation exists. Here, as can be seen from figures 1 and 2, the speed of particles never drops to zero for $q > 0$. In our model the presence of a single negative particle produces a macroscopic shock for $q \leqslant q_c$. In the power-law phase $q \geqslant q_c$ the density profile of positive particles has an exponential behaviour with correlation length ξ which diverges at the transition point. This implies a second-order phase transition at this point.

The next step could be analytical study of this model with unequal but finite densities of positive ρ_+ and negative particles ρ_-. An approach can be considering the model with open boundaries where the injection and extraction rates control the bulk density. Work in this direction is in progress [12].

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Appendix. Formulas for $Z_{L,M}$, V_+ and V_-

In the following we show that the normalization factor $Z_{L,M}$ can be calculated directly using the algebra (3)–(5). First, we note that one can split (6) into two terms as

$$Z_{L,M} = \mathrm{Tr}(G_{L-1,M}EA) + \mathrm{Tr}(G_{L-1,M-1}DA). \tag{15}$$

Now using (4) and (5) it is not difficult to see that (15) can be written as

$$Z_{L,M} = C^{M}_{L-2}\,\mathrm{Tr}(E^{L-M-1}A) + \mathrm{Tr}(G_{L-1,M-1}DA). \tag{16}$$

This can be done by noting that the first term in (15) can be written as

$$\begin{aligned}\mathrm{Tr}(G_{L-1,M}EA) &= \mathrm{Tr}\left(\sum_{\{\tau_i=0,1\}}\delta\left(M-\sum_{i=1}^{L-2}\tau_i\right)\prod_{i=1}^{L-2}(\tau_i D + (1-\tau_i)E)EA\right)\\ &= \sum_{\{\tau_i=0,1\}}\delta\left(M-\sum_{i=1}^{L-2}\tau_i\right)\mathrm{Tr}\left(\prod_{i=1}^{L-2}(\tau_i D + (1-\tau_i)E)EA\right)\\ &= \sum_{\{\tau_i=0,1\}}\delta\left(M-\sum_{i=1}^{L-2}\tau_i\right)\mathrm{Tr}(E^{L-M-2}EA)\end{aligned}$$

which gives the first term in (16). One can expand the second term in (16) repeatedly as follows:

$$\begin{aligned}\mathrm{Tr}(G_{L-1,M-1}DA) &= \mathrm{Tr}(G_{L-2,M-1}EDA) + \mathrm{Tr}(G_{L-2,M-2}DDA)\\ &= C^{M-1}_{L-3}\,\mathrm{Tr}(E^{L-M-2}DA) + \mathrm{Tr}(G_{L-2,M-2}D^2A)\end{aligned}$$

to obtain the following compact formula for the partition function:

$$Z_{L,M} = \sum_{i=0}^{M}\mathrm{Tr}(E^{L-M-1}D^iA)C^{M-i}_{L-i-2}. \tag{17}$$

The expression (17) can easily be calculated using the algebra (3)–(5)

$$\begin{aligned}f_i \equiv \mathrm{Tr}(E^{L-M-1}D^iA) &= \mathrm{Tr}\left(E^{L-M-1}D^{i-1}\frac{1}{q}(AD+A+D)\right)\\ &= \frac{1}{q}(2f_{i-1} + \mathrm{Tr}(E^{L-M-1})).\end{aligned}$$

Solving the above difference equation gives

$$f_i = \frac{(q-3)(\frac{2}{q})^i + 1}{q-2} \operatorname{Tr}(E^{L-M-1}) \quad i = 0, \ldots, M. \tag{18}$$

Since $Z_{L,M}$ enters both denominator and numerator of physical quantities, the same common factor $\operatorname{Tr}(E^{L-M-1})$ cancels from all formulae so the results are independent of its value. For simplicity we set $\operatorname{Tr}(E^{L-M-1}) = 1$.

The current of the positive particles is defined as

$$J_+ = P(\tau_i = 1, \tau_{i+1} = 0) + qP(\tau_i = 1, \tau_{i+1} = 2) - P(\tau_{i+1} = 1, \tau_i = 2) \tag{19}$$

in which $P(\tau_i = m, \tau_j = n)$ is the probability of finding the system in configuration $\{C\}$ provided that a particle of kind m is at site i and a particle of kind n at site j. Now we can write (19) in terms of the conditional probability (2) as follows:

$$\begin{aligned} J_+ &= P(\tau_i = 1, \tau_{i+1} = 0) + qP(\tau_i = 1|\tau_{i+1} = 2)P(\tau_{i+1} = 2) \\ &\quad - P(\tau_{i+1} = 1|\tau_i = 2)P(\tau_i = 2) \\ &= P(\tau_i = 1, \tau_{i+1} = 0) + \frac{1}{L}\left(q\frac{\operatorname{Tr}(G_{L-1,M-1}DA)}{\operatorname{Tr}(G_{L,M}A)} - \frac{\operatorname{Tr}(G_{L-1,M-1}AD)}{\operatorname{Tr}(G_{L,M}A)}\right) \end{aligned}$$

in which we have used $P(\tau_i = 2) = \frac{1}{L}$. Using the algebra (3)–(5) we obtain

$$\begin{aligned} J_+ &= P(\tau_i = 1, \tau_{i+1} = 0) + \frac{1}{L}\frac{\operatorname{Tr}(G_{L-2,M-1}(A+D))}{\operatorname{Tr}(G_{L,M}A)} \\ &= P(\tau_i = 1, \tau_{i+1} = 0) + \frac{1}{L}\frac{Z_{L-1,M-1} + C_{L-2}^{M-1}}{Z_{L,M}} \end{aligned} \tag{20}$$

in which we have $\operatorname{Tr}(G_{L-2,M-1}A) = Z_{L-1,M-1}$ and

$$\begin{aligned} \operatorname{Tr}(G_{L-2,M-1}D) &= \sum_{\{\tau_i=0,1\}} \delta\left(M - 1 - \sum_{i=1}^{L-2}\tau_i\right) \operatorname{Tr}\left(\prod_{i=1}^{L-2}(\tau_i D + (1-\tau_i)E)D\right) \\ &= \sum_{\{\tau_i=0,1\}} \delta\left(M - 1 - \sum_{i=1}^{L-2}\tau_i\right) \operatorname{Tr}(E^{L-M-2}) = C_{L-2}^{M-1}. \end{aligned}$$

The first term in (20) can be written as

$$\begin{aligned} P(\tau_i = 1, \tau_{i+1} = 0) &= \sum_{k=1, k\neq i,i+1}^{L} P(\tau_i = 1, \tau_{i+1} = 0|\tau_k = 2)P(\tau_k = 2) \\ &= \frac{1}{L}\sum_{k=2}^{L-1} P(\tau_k = 1, \tau_{k+1} = 0|\tau_1 = 2) = \frac{1}{L}\sum_{k=2}^{L-1}\sum_{p=0}^{M-1}\frac{\operatorname{Tr}(G_{j,p}DEG_{L-j-1,M-p}A)}{\operatorname{Tr}(G_{L,M}A)} \\ &= \frac{(L-M-1)Z_{L-1,M-1}}{LZ_{L,M}}. \end{aligned}$$

Putting the last term in (20) gives

$$J_+ = \frac{(L-M)Z_{L-1,M-1} + C_{L-2}^{M-1}}{LZ_{L,M}}.$$

Now we can calculate the speed of the positive particles

$$V_+ = \frac{L}{M}J_+ = \frac{(L-M)Z_{L-1,M-1} + C_{L-2}^{M-1}}{MZ_{L,M}} \tag{21}$$

which is exactly expression (8). The speed of the negative particle is also defined as follows:

$$V_- = P(\tau_i = 0|\tau_{i+1} = 2) + qP(\tau_i = 1|\tau_{i+1} = 2) - P(\tau_{i+1} = 1|\tau_i = 2).$$

Now using the expression (2) for the conditional probability and the algebra (3)–(5) we obtain

$$\begin{aligned} V_- &= \frac{\mathrm{Tr}(G_{L-1,M}EA)}{\mathrm{Tr}(G_{L,M}A)} + q\frac{\mathrm{Tr}(G_{L-1,M}DA)}{\mathrm{Tr}(G_{L,M}A)} - \frac{\mathrm{Tr}(G_{L-1,M}AD)}{\mathrm{Tr}(G_{L,M}A)} \\ &= \frac{\mathrm{Tr}(G_{L-1,M}EA)}{\mathrm{Tr}(G_{L,M}A)} + \frac{Z_{L-1,M-1} + C_{L-2}^{M-1}}{Z_{L,M}} = \frac{Z_{L-1,M-1} + C_{L-2}^{M} + C_{L-2}^{M-1}}{Z_{L,M}}. \end{aligned} \tag{22}$$

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